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Ferro- and Antiferroelectric Substances

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**7 Layer-structure oxides****7A Pure compounds of simple type****Nr. 7A-1 Bi<sub>3</sub>TiNbO<sub>9</sub>**

1a	Dielectric anomaly associated with a phase transition was reported by ISMAILZADE in 1960.			60I1
b	phase	II	I	
	state		P <sup>a)</sup>	
	crystal system	orthorhombic <sup>b)</sup>	tetragonal <sup>b)</sup>	
	space group	Fmm2-C <sub>4v</sub> <sup>16</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	Θ*	900 ... 950 °C <sup>b)</sup>		
		$\rho = 6.4 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 5.40 \text{ Å}, b = 5.44 \text{ Å}, c = 25.1 \text{ Å}$ at RT.		
4	Temperature dependence of lattice parameters: Fig. 868. Linear thermal expansion: Fig. 869.			
5a	Dielectric constant: Fig. 870. $\approx 100$ at RT. The dielectric constant was not measured in the vicinity of the transition point because of high conductivity. Extrapolation of the Curie temperatures of the solid solution system obtained by the dielectric measurements indicates a transition temperature between 900° and 950 °C for Bi <sub>3</sub> TiNbO <sub>9</sub> .			61S11

**Nr. 7A-2 Bi<sub>3</sub>TiTaO<sub>9</sub>**

1a	Phase transition similar to that of Bi <sub>3</sub> TiNbO <sub>9</sub> was reported by SUBBARAO in 1962.			62S17
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	space group	Fmm2-C <sub>4v</sub> <sup>16</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	Θ	870 °C		
		$\rho = 8.5 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 5.39 \text{ Å}, b/a = 1.007, c = 25.1 \text{ Å}$ at RT.		
4	Linear thermal expansion: see Fig. 869.			
5a	Dielectric constant: $\approx 140$ at RT.			62S17

**Nr. 7A-3 CaBi<sub>3</sub>Nb<sub>2</sub>O<sub>9</sub>**

1a	Dielectric anomaly associated with a phase transition was discovered by ISMAILZADE in 1960.			60I1
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	space group	Fmm2-C <sub>4v</sub> <sup>16</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	Θ	625 °C		
		$\rho = 5.0 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 5.39 \text{ Å}, b/a = 1.006, c = 25.15 \text{ Å}$ at RT.		
4	Temperature dependence of lattice parameters: Tab. 104.			
5a	Dielectric constant: Fig. 871. $\approx 80$ at RT.			62S17

\* According to [60I1] Θ is 600 ... 650 °C.

Tab. 104. Temperature dependence of the lattice parameters of  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{CaBi}_2\text{Ta}_2\text{O}_9$  [60I1]

T	20	100	150	200	250	300	350	400	°C
$\text{CaBi}_2\text{Nb}_2\text{O}_9$									
a	5.442	—	5.453	—	5.458	—	5.465	—	Å
b	5.482 <sub>b</sub>	—	5.484	—	5.487	—	5.491	—	Å
c	24.920	—	24.955	—	24.990	—	25.035	—	Å
b/a	1.0075	—	1.0056	—	1.005 <sub>b</sub>	—	1.0047	—	Å
V	743.5	—	746.0	—	748.5	—	751.0	—	Å <sup>3</sup>
$\text{CaBi}_2\text{Ta}_2\text{O}_9$									
a	5.435	5.438	—	5.444	—	5.452	—	5.464	Å
b	5.468 <sub>b</sub>	5.471	—	5.475 <sub>b</sub>	—	5.479	—	5.482 <sub>b</sub>	Å
c	24.970	24.980	—	25.015	—	25.040	—	25.060	Å
b/a	1.006	1.006	—	1.005 <sub>b</sub>	—	1.005	—	1.003 <sub>b</sub>	Å
V	742.0	743.2	—	745.6	—	748.0	—	750.6	Å <sup>3</sup>
T	450	500	550	575	600	650	700	—	°C
$\text{CaBi}_4\text{Nb}_2\text{O}_9$									
a	5.480	5.485	5.488 <sub>b</sub>	5.495 <sub>b</sub>	—	5.502 <sub>b</sub>	5.504	—	Å
b	5.496 <sub>b</sub>	5.501 <sub>b</sub>	5.502 <sub>b</sub>	5.503 <sub>b</sub>	—	5.502 <sub>b</sub>	5.504	—	Å
c	25.070	25.080	25.090	25.105	—	25.125	25.140	—	Å
b/a	1.0036	1.0029	1.0025	1.0015	—	1.000	1.000	—	Å
V	755.0	756.8	758.0	759.3	—	760.7	761.6	—	Å <sup>3</sup>
$\text{CaBi}_4\text{Ta}_2\text{O}_9$									
a	—	5.470	5.473	—	5.479	5.484	—	—	Å
b	—	5.483 <sub>b</sub>	5.484	—	5.479	5.484	—	—	Å
c	—	25.070	25.083	—	25.085	25.105	—	—	Å
b/a	—	1.002 <sub>b</sub>	1.002 <sub>b</sub>	—	1.000	1.000	—	—	Å
V	—	751.9	752.8	—	730.0	755.0	—	—	Å <sup>3</sup>

Nr. 7A-4  $\text{CaBi}_2\text{Ta}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by ISMAILZADE in 1960.	60I1
b	phase state crystal system space group $\Theta$	II P orthorhombic Fmm2-C <sub>4v</sub> <sup>18</sup> 575 °C
		5.428 Å, $b/a = 1.006, c = 24.90 \text{ \AA}$ at RT.
4	Temperature dependence of lattice parameter: see Tab. 104.	60I1 61S11
5a	Dielectric constant: Fig. 872.	
Nr. 7A-5 $\text{SrBi}_2\text{Nb}_2\text{O}_9$		
1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.	61S11
b	phase state crystal system $\Theta$	II P orthorhombic 420 °C
		$e = 6.9 \cdot 10^3 \text{ kg m}^{-3}\text{s}^{-1}$ , $a = 5.506 \text{ \AA}, b/a = 1.000, c = 25.05 \text{ \AA}$ at RT.
5a	Dielectric constant: Fig. 873. $\propto \approx 190$ at RT. $\propto = C/(T - \Theta_p)$ , where $C = 0.55 \cdot 10^5 \text{ ^\circ C}$ , $\Theta_p = 390 \text{ ^\circ C}$ .	62S15 62S17
7a	Piezoelectricity: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$	62S17

Nr. 7A-6 $\text{SrBi}_3\text{Ta}_2\text{O}_9$							
1a	Ferroelectricity in $\text{SrBi}_3\text{Ta}_2\text{O}_9$ was reported by SMOLENSKII in 1961.						
b	phase	II	I				
	state	F	P				
	crystal system	orthorhombic	tetragonal				
	$\Theta$	310 °C					
	$\rho$	$7.5 \cdot 10^3 \text{ kg m}^{-3}$ .					
	$a$	$a = 5.512 \text{ \AA}, b/a = 1.000, c = 25.00 \text{ \AA}$ at RT.					
5a	Dielectric constant: Fig. 874. $\kappa \approx 180$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 2.0 \cdot 10^6 \text{ }^\circ\text{C}$ , $\Theta_p = 190 \text{ }^\circ\text{C}$ .						
c	Spontaneous polarization: $P_s = 5.8 \cdot 10^{-2} \text{ C m}^{-2}$ at 25 °C.						
7a	Piezoelectric constant: $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .						
Nr. 7A-7 $\text{BaBi}_3\text{Nb}_2\text{O}_9$							
1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.						
b	phase	II	I				
	state		P				
	crystal system	orthorhombic	tetragonal				
	$\Theta$	210 °C					
		200 <sup>a</sup> ) °C					
	$\rho$	$6.3 \cdot 10^3 \text{ kg m}^{-3}$ .					
	$a$	$a = 5.554 \text{ \AA}, b/a = 1.000, c = 25.60 \text{ \AA}$ at RT.					
5a	Dielectric constant: Fig. 875. $\kappa = 280$ at RT.						
Nr. 7A-8 $\text{BaBi}_3\text{Ta}_2\text{O}_9$							
1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.						
b	phase	II	I				
	state		P				
	crystal system	orthorhombic	tetragonal				
	$\Theta$	110 <sup>a</sup> ) °C					
	According to [61S11] $\Theta$ is 70 °C.						
	$\rho$	$8.4 \cdot 10^3 \text{ kg m}^{-3}$ .					
	$a$	$a = 5.556 \text{ \AA}, b/a = 1.000, c = 25.50 \text{ \AA}$ at RT.					
5a	Dielectric constant: Fig. 876. $\kappa = 400$ at RT.						
Nr. 7A-9 $\text{PbBi}_3\text{Nb}_2\text{O}_9$							
1a	Dielectric anomaly associated with a phase transition in $\text{PbBi}_3\text{Nb}_2\text{O}_9$ was reported by SMOLENSKII in 1959.						
b	phase	II	I				
	state		P				
	crystal system	orthorhombic	tetragonal				
	$\Theta$	526 °C					
		550 <sup>a</sup> ) °C					
	$\rho$	$7.6 \cdot 10^3 \text{ kg m}^{-3}$ .					
	$a$	$a = 5.488 \text{ \AA}, b/a = 1.002, c = 25.55 \text{ \AA}$ at RT.					
3	Crystal structure: Fig. 877.						
4	Temperature dependence of lattice parameters: Fig. 878.						
5a	Dielectric constant: Fig. 879. $\kappa = 170$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 1.3 \cdot 10^6 \text{ }^\circ\text{K}$ , $\Theta_p = 510 \text{ }^\circ\text{C}$ .						
7a	Piezoelectric constant: $d_{33} = 1.5 \cdot 10^{-11} \text{ C N}^{-1}$ .						

## Figuren S. 377ff.

## II 7 Oxide mit Schichtstruktur

Nr. 7A-10  $\text{PbBi}_3\text{Ta}_2\text{O}_9$ 

1a	Ferroelectricity was reported by SUBBARAO <sup>a)</sup> and SMOLENSKIR <sup>b)</sup> independently in 1961.	<sup>a) 61S15 b) 61S11</sup>
b	phase      II      I	
state	F	P
crystal system	orthorhombic	tetragonal
$\Theta$	430 °C	
$\rho = 9.0 \cdot 10^3 \text{ kg m}^{-3}$		
$a = 5.496 \text{ \AA}, b/a = 1.000, c = 25.40 \text{ \AA}$ at RT.		
5a	Dielectric constant: Fig. 880. $\kappa = 180$ at RT. $\kappa = C/(T - \Theta_p), C = 3.7 \cdot 10^4 \text{ ^\circ C}, \Theta_p = 325 \text{ ^\circ C}$ .	62S17
7a	Piezoelectric constant: $d_{33} = 5 \cdot 10^{-12} \text{ C N}^{-1}$ .	62S17

Nr. 7A-11  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ 

1a	Ferroelectricity in $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ was reported by VAN UITERT et al. in 1961.	61V2
b	phase      II      I	
state	F	P
crystal system	monoclinic*) (pseudo-orthorhombic)	tetragonal
$\Theta$	675 °C	
	Unit cell is very nearly orthorhombic with the lattice parameters: $a_{\text{orth}} = 5.411 \text{ \AA}$ , $b_{\text{orth}} = 5.448 \text{ \AA}, c_{\text{orth}} = 32.85 \text{ \AA}$ at RT. Relations between crystallographic axes: Fig. 881. $P_3$ lies in a direction tilted at approximately 7° (or less) from the major crystal surface in a plane parallel to the pseudo-orthorhombic $b - c$ plane.	
2a	Crystal growth: Cooling method from melt consisting of 100 $\text{Bi}_4\text{O}_7$ and 5 $\text{TiO}_2$ (weight ratio).	61V2
3	Crystal structure: Fig. 882.	
4	Temperature dependence of lattice parameter: Fig. 883. Thermal expansion: Fig. 884.	
5a	Dielectric constant: Fig. 885.	
c	$P_s$ and $E_s$ : Fig. 886, 887. TAMBOVTSEV et al. measured $P_s$ and $E_s$ by applying a field parallel to the $c_{\text{orth}}$ direction, $P_s = 1.99 \cdot 10^{-2} \text{ C m}^{-2}$ , $E_s = 1.13 \cdot 10^4 \text{ V m}^{-1}$ . According to [67C6], the spontaneous polarization lies in the pseudo-orthorhombic (100) plane and has a value larger than $30 \cdot 10^{-3} \text{ C m}^{-2}$ .	63T1 67C6
7	Piezoelectric constant: $d_{33} = 2.0 \cdot 10^{-11} \text{ C N}^{-1}$ .	61S17
10	Conductivity: see	64P3
14a	Domain structure: see Domains have been observed by polarized light.	64P3 66C7
b	Switching: Fig. 888, 889. See also Fig. 892, Tab. 105 and:	66P6
17	Twinning structure: see	64P3

Nr. 7A-12  $\text{BaBi}_3\text{Ti}_5\text{NbO}_{12}$ 

1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.	61S15
b	phase      II      I	
state		P
crystal system	pseudo-tetragonal	tetragonal
$\Theta$	270 °C	
	$a = 3.874 \text{ \AA}, c = 33.70 \text{ \AA}$ at RT.	

Nr. 7A-13  $\text{PbBi}_3\text{Ti}_5\text{NbO}_{12}$ 

1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.	61S15
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\* Point group is m.

1b	phase	II	I	
	state		P	
	crystal system	pseudo-tetragonal	tetragonal	
	$\Theta$	290 °C		61S15 61S15

$a = 3.687 \text{ \AA}$ ,  $c = 33.55 \text{ \AA}$  at RT.

Nr. 7A-14  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ 

1a	Dielectric anomaly associated with a phase transition was reported independently by SUBBARAO <sup>a</sup> ) and by SMOLENSKII <sup>b</sup> ) in 1961. Ferroelectric activity was reported independently by FANG et al. in 1961 <sup>c</sup> ).			
	phase	II	I	
	state	F	P	61F7
	crystal system	orthorhombic (or pseudo-orthorhombic)	tetragonal	

$\Theta$       375 °C  
 $\Theta$       395<sup>a</sup> °C

$\rho = 5.7 \cdot 10^8 \text{ kg m}^{-3}$   
 $a = 5.461 \text{ \AA}$ ,  $b/a = 1.000$ ,  $c = 41.85 \text{ \AA}$  at RT.

<sup>a</sup>) 61S15  
62S15

## 3 Crystal structure: Fig. 890.

## 5a Dielectric constant: Fig. 891.

 $\kappa = C/(T - \Theta_p)$ ,  $C = 2.5 \cdot 10^5 \text{ }^\circ\text{K}$ ,  $\Theta_p = 335 \text{ }^\circ\text{C}$ .

61S15

7a Piezoelectric constant:  $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .

62S17

## 14b Switching: Fig. 892; Tab. 105.

Tab. 105.  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ ,  $\text{Ba}_2\text{Bi}_4\text{Ti}_4\text{O}_{18}$ ,  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ ,  $\text{BaTiO}_3$  (for comparison). Switching parameters in comparison with those of  $\text{BaTiO}_3$  [62F1].  $t_s = t_\infty \exp(+\alpha/E)$ ,  $t_s$  = switching time

	$\text{BaTiO}_3$	$\text{Bi}_4\text{Ti}_3\text{O}_{12}$	$\text{BaBi}_4\text{Ti}_4\text{O}_{15}$	$\text{Ba}_2\text{Bi}_4\text{Ti}_4\text{O}_{18}$	
$\alpha$	6.1	41	23	76	$10^5 \text{ V m}^{-1}$
$t_\infty$	0.4	$10^{-2}$	1.5	$10^{-3}$	$\mu \text{ sec}$

Nr. 7A-15  $\text{PbBi}_4\text{Ti}_4\text{O}_{15}$ 

1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.	61S15
	phase	II
	state	P
	crystal system	orthorhombic (possibly)

$\Theta$       570 °C

$\rho = 6.6 \cdot 10^8 \text{ kg m}^{-3}$   
 $a = 5.437 \text{ \AA}$ ,  $b/a = 1.000$ ,  $c = 41.35 \text{ \AA}$  at RT.

<sup>a</sup>) 62S15

## 5a Dielectric constant: Fig. 893.

 $\kappa = C/(T - \Theta_p)$ ,  $C = 1.4 \cdot 10^5 \text{ }^\circ\text{C}$ ,  $\Theta_p = 552 \text{ }^\circ\text{C}$ .61S15  
62S177a Piezoelectric constant:  $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .

62S17

Nr. 7A-16  $\text{SrBi}_4\text{Ti}_4\text{O}_{15}$ 

1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.	61S15
	phase	II
	state	P
	crystal system	orthorhombic (possibly)

$\Theta$       530 °C

$\rho = 5.2 \cdot 10^8 \text{ kg m}^{-3}$   
 $a = 5.428 \text{ \AA}$ ,  $b/a = 1.000$ ,  $c = 40.95 \text{ \AA}$  at RT.

<sup>a</sup>) 62S17  
62S15

## 5a Dielectric constant: Fig. 894.

 $\kappa = C/(T - \Theta_p)$ ,  $C = 0.68 \cdot 10^5 \text{ }^\circ\text{C}$ ,  $\Theta_p = 485 \text{ }^\circ\text{C}$ .

62S17

7a Piezoelectric constant:  $d_{33} = 1.5 \cdot 10^{-11} \text{ C N}^{-1}$ .

62S17

Nr. 7A-17  $\text{CaBi}_4\text{Ti}_4\text{O}_{15}$ 

1a	$\text{CaBi}_4\text{Ti}_4\text{O}_{15}$ was investigated by SUBBARAO in 1962. No dielectric anomaly has been detected.	62S17
b	Orthorhombic: $a = 5.418 \text{ \AA}$ , $b/a = 1.002$ , $c = 40.75 \text{ \AA}$ at RT. $\rho = 4.7 \cdot 10^3 \text{ kg m}^{-3}$ .	62S15
5a	Dielectric constant: Fig. 895. $\kappa = 120$ at RT.	61S11

Nr. 7A-18  $\text{Bi}_5\text{Ti}_3\text{GaO}_{15}$ 

1a	$\text{Bi}_5\text{Ti}_3\text{GaO}_{15}$ was investigated by SUBBARAO in 1962. No dielectric anomaly has been detected.	62S17
b	Orthorhombic: $a = 5.408 \text{ \AA}$ , $b/a = 1.006$ , $c = 41.05 \text{ \AA}$ at RT. $\rho = 7.3 \cdot 10^3 \text{ kg m}^{-3}$ .	62S15
5a	Dielectric constant: $\kappa = 150$ at RT.	62S17

Nr. 7A-19  $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ 

1a	Ferroelectric activity of $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by AURIVILLIUS in 1962.	62A5
b	phase II I state F P crystal system orthorhombic tetragonal $\Theta = 325^\circ \text{ C}$ $a = 5.527 \text{ \AA}$ , $b = 5.514 \text{ \AA}$ , $c = 50.37 \text{ \AA}$ at RT.	62A5 63I5
3	Crystal structure: Fig. 896; Tab. 106.	
4	Temperature dependence of lattice parameter: Fig. 897.	
5a	Dielectric constant: Fig. 898. $\kappa' = 360$ , $\kappa'' = 22$ at RT.	62A5
c	Remanent polarization: $P_r = 2 \cdot 10^{-8} \text{ C m}^{-2}$ at RT. Coercive field: $E_c = 1.0 \cdot 10^6 \text{ V m}^{-1}$ at RT.	62A5
14b	Switching: see Fig. 892; Tab. 105.	

Tab. 106.  $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ . Fractional coordinates of atoms [62A5]. Space group of I4/mmm was assumed.

I4/mmm	(0, 0, 0; 1/2, 1/2, 1/2) +	
4 Bi in 4(e):	$\pm 0, 0, z$ :	$z = 0.2255$
4 (Bi, Ba) in 4(e):		$z = 0.0420$
4 (Bi, Ba) in 4(e):		$z = 0.1300$
2 Ti in 2(b):	$\pm 0, 0, 1/2$	
4 Ti in 4(e):		$z = 0.3370$
4 Ti in 4(e):		$z = 0.4185$
4 O in 4(c):	0, 1/2, 0; 1/2, 0, 0	
4 O in 4(d):	0, 1/2, 1/4; 1/2, 0, 1/4	
4 O in 4(e):		$z = 0.2962$
4 O in 4(e):		$z = 0.3378$
4 O in 4(e):		$z = 0.4593$
8 O in 8(g):	$\pm (0, 1/2, z; 1/2, 0, z)$	$z = 0.0815$
8 O in 8(g):		$z = 0.1630$

Nr. 7A-20  $\text{Pb}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ 

1a	Ferroelectric activity in $\text{Pb}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by SUBBARAO in 1962.	62S17
b	phase II I state F P crystal system orthorhombic (possibly) tetragonal $\Theta = 310^\circ \text{ C}$ $\rho = 6.6 \cdot 10^3 \text{ kg m}^{-3}$ . $a = 5.461 \text{ \AA}$ , $b/a = 1.000$ , $c = 49.70 \text{ \AA}$ at RT.	62S17 62S15

5a	Dielectric constant: Fig. 899. $\kappa = 400$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 4.1 \cdot 10^6$ °K, $\Theta_p = 280$ °C.	62S17
c	Spontaneous polarization: $P_s = 6 \cdot 10^{-2}$ C m <sup>-2</sup> at 235 °C.	62S17
7a	Piezoelectric constant: $d_{33} = 2.5 \cdot 10^{-12}$ C N <sup>-1</sup> .	62S17

Nr. 7A-21  $\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ 

1a	Ferroelectric activity in $\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by SUBBARAO in 1962.	62S17
b	phase                    II                    I state                    F                    P crystal system            orthorhombic            tetragonal $\Theta$ 285 °C $\rho = 5.3 \cdot 10^3$ kg m <sup>-3</sup> . $a = 5.461$ Å, $b/a = 1.000$ , $c = 48.80$ Å at RT.	62S17 62S15
5a	Dielectric constant: Fig. 900. $\kappa = 280$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 0.47 \cdot 10^5$ °K, $\Theta_p = 255$ °C.	62S17
c	Spontaneous polarization: $P_s = 3.5 \cdot 10^{-3}$ C m <sup>-2</sup> at 255 °C.	62S17
7a	Piezoelectric constant: $d_{33} = 2.5 \cdot 10^{-12}$ C N <sup>-1</sup> .	62S17

Nr. 7A-22  $\text{Bi}_2\text{Ti}_4\text{O}_{11}$ 

1a	Dielectric anomaly associated with a phase transition was observed in $\text{Bi}_2\text{Ti}_4\text{O}_{11}$ by SUBBARAO in 1962.	62S16
b	phase                    III                    II                    I crystal system            monoclinic            monoclinic            — space group              C2/c-C <sub>2h</sub> <sup>+</sup> C2/m-C <sub>2h</sub> <sup>+</sup> — $\Theta$ 250° <sup>a</sup> 1200° <sup>a</sup> °C $\rho = (6.12 \pm 0.02) \cdot 10^3$ kg m <sup>-3</sup> . $a = (14.612 \pm 0.006)$ Å, $b = (3.799 \pm 0.004)$ Å, $c = (14.946 \pm 0.006)$ Å, $\beta = (93.13 \pm 0.01)$ ° at RT.	65J4 *)62S16 65J4 65J4
3	Crystal structure: $Z = 2$ in phase II. $Z = 4$ in phase III. Fig. 901, 902; Tab. 107.	65J4
4	Thermal expansion: Fig. 903.	
5a	Dielectric constant: Fig. 904.	
c	No hysteresis loops could be obtained between 25 °C and 290 °C.	62S16

Tab. 107.  $\text{Bi}_2\text{Ti}_4\text{O}_{11}$ . Atomic parameters at RT [65J4]

Atom	x	y	z
O(1)	0.0	0.262 $\pm$ 0.012	0.250
O(2)	0.1828 $\pm$ 0.0024	0.246 $\pm$ 0.007	0.2207 $\pm$ 0.0024
O(3)	0.1408 $\pm$ 0.0024	0.256 $\pm$ 0.007	0.0338 $\pm$ 0.0024
O(4)	0.0814 $\pm$ 0.0024	0.760 $\pm$ 0.007	0.1259 $\pm$ 0.0024
O(5)	0.2662 $\pm$ 0.0024	0.747 $\pm$ 0.007	0.0880 $\pm$ 0.0024
O(6)	0.0546 $\pm$ 0.0024	0.770 $\pm$ 0.007	0.9221 $\pm$ 0.0024
Ti(1)	0.0530 $\pm$ 0.0006	0.250 $\pm$ 0.002	0.1406 $\pm$ 0.0006
Ti(2)	0.1461 $\pm$ 0.0006	0.759 $\pm$ 0.002	0.0162 $\pm$ 0.0006
Bi	0.3211 $\pm$ 0.00015	0.1747 $\pm$ 0.0005	0.1798 $\pm$ 0.00015

Thermal parameter  $B = 0.33$  Å<sup>2</sup> for all atoms. Coordinates and standard deviations in cell fractions.

## 7B Complex compounds and solid solutions

Nr. 7B-1 $\text{Bi}_{8-x}\text{Me}_x^{2+}\text{Ti}_{1-x}\text{Nb}_{1+x}\text{O}_9$ ( $\text{Me}^{2+} = \text{Ba}, \text{Sr}, \text{Pb}$ )	1b	Lattice parameter: Fig. 905. Transition temperature: Fig. 906.
	5	Dielectric constant: Fig. 907.
Nr. 7B-2 $\text{Bi}_{4-x}\text{Me}_x^{2+}\text{Ti}_{4-x}\text{Nb}_x\text{O}_{11}$ ( $\text{Me}^{2+} = \text{Ba}, \text{Sr}, \text{Pb}$ )	1b	Lattice parameter: Fig. 908. Transition temperature: Fig. 909.
	5	Dielectric constant: Fig. 910.

\* The unit cell of phase II has about half the volume of the unit cell of phase III.

<b>Nr. 7B-3 <math>\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}</math></b>					
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1962.				
b	phase	II	I		
	state		P		
	crystal system	orthorhombic	tetragonal		
	$\Theta$	650 °C			
	$\epsilon = 6.3 \cdot 10^8 \text{ kg m}^{-3}$ .				
	$a = 5.427 \text{ \AA}$ , $b/a = 1.006$ , $c = 40.65 \text{ \AA}$ at RT.				
5a	Dielectric constant: Fig. 911. $x = 200$ at RT. $x = C/(T - \Theta_p)$ , $C = 0.79 \cdot 10^5 \text{ °K}$ , $\Theta_p = 610 \text{ °C}$ .				
7a	Piezoelectric constant: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$ .				
<b>Nr. 7B-4 <math>\text{K}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}</math></b>					
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1962.				
b	phase	II	I		
	state		P		
	crystal system	orthorhombic	tetragonal		
	$\Theta$	550 °C			
	$\epsilon = 6.7 \cdot 10^8 \text{ kg m}^{-3}$ .				
	$a = 5.440 \text{ \AA}$ , $b/a = 1.004$ , $c = 41.15 \text{ \AA}$ at RT.				
5a	Dielectric constant: Fig. 912. $x = 140$ at RT. $x = C/(T - \Theta_p)$ , $C = 0.74 \cdot 10^5 \text{ °K}$ , $\Theta_p = 515 \text{ °C}$ .				
7a	Piezoelectric constant: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$ .				
<b>Nr. 7B-5 <math>(\text{Pb}_{1-x}\text{Ba}_x)\text{Bi}_4\text{Nb}_2\text{O}_9</math> and <math>(\text{Pb}_{1-x}\text{Sr}_x)\text{Bi}_4\text{Nb}_2\text{O}_9</math></b>					
1b	Transition temperature: Fig. 913.				
5	Dielectric constant: Fig. 914.				
<b>Nr. 7B-6 <math>(1-x)\text{Bi}_4\text{Ti}_4\text{O}_{15} - x\text{BaTiO}_3</math></b>					
5	Transition temperature: Fig. 915.				
<b>Nr. 7B-7 <math>\text{Bi}_{4+x}\text{Pb}_{1-x}\text{Ti}_{4-x}\text{Ga}_x\text{O}_{15}</math></b>					
1a	Another formula for this solid solution is $(1 - x)\text{PbBi}_4\text{Ti}_4\text{O}_{15} \cdot x\text{Bi}_5\text{Ti}_3\text{GaO}_{15}$ . Properties of this solid solution were studied by SUBBARAO in 1962.				
b	$x = 0.25$ :				
	phase	II	I		
	state		P		
	crystal system	orthorhombic (pseudo-tetragonal)	tetragonal		
	$\Theta$	600 °C			
	Pseudo-tetragonal cell parameter: $a = 3.842 \text{ \AA}$ , $c = 41.40 \text{ \AA}$ at RT. Dielectric constant: $x = 180$ at RT; $x = 3035$ at $\Theta$ .				
	$x = 0.5$ :				
	phase	II	I		
	state		P		
	crystal system	orthorhombic (pseudo-tetragonal)	tetragonal		
	$\Theta$	620 °C			
	Pseudo-tetragonal cell parameter: $a = 3.842 \text{ \AA}$ , $c = 41.40 \text{ \AA}$ at RT. Dielectric constant: $x = 179$ at RT; $x = 1930$ at $\Theta$ .				